Tubular reactor (PDE modes)

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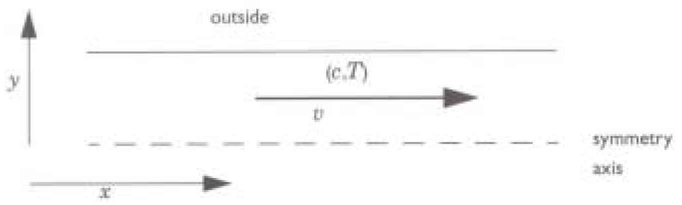
Tubular reactor
(Scaled equation)

- Cooling effect of the walls in a cylindrical reactor. Considering these effects, the scaled equations are as follows.



$$\frac{\partial T}{\partial t} + r_2 \frac{\partial T}{\partial x^2} = r_0 \frac{\partial^2 T}{\partial x^2} + r_0 \frac{L_R}{y} \frac{\partial}{\partial y}\left(y \frac{\partial T}{\partial y}\right) + B_1 c e^{-\frac{q}{T}}$$

$$\frac{\partial c}{\partial t} + r_2 \frac{\partial c}{\partial x^2} = r_0 \frac{\partial^2 c}{\partial x^2} + \frac{L_R}{y} \frac{\partial}{\partial y}\left(y \frac{\partial c}{\partial y}\right) - B_2 e^{-\frac{q}{T}}$$

Tubular reactor (Boundary conditions)

$$-r_0 \frac{\partial T}{\partial x}(0,y,t) = r_2(T_0 - T(0,y,t)) \qquad \frac{\partial T}{\partial x}(1,y,t) = 0$$

$$-\frac{\partial c}{\partial x}(0,y,t) = r_2(c_0 - c(0,y,t)) \qquad \frac{\partial c}{\partial x}(1,y,t) = 0$$

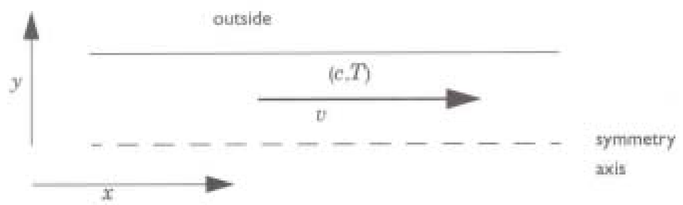
$$\frac{\partial T}{\partial y}(x,0,t) = 0 \qquad \frac{\partial T}{\partial y}(x,1,t) = \kappa(T_R - T(x,1,t))$$

$$\frac{\partial c}{\partial y}(x,0,t) = 0 \qquad \frac{\partial c}{\partial y}(x,1,t) = 0$$

$$T = T(x,y,t), \quad c = c(x,y,t)$$

Parameter	Meaning
T_R	Scaled temperature
L_R	Scaled radius
κ	Scaled heat transfer coefficient

Model : Cylindrical tubular reactor with cooling



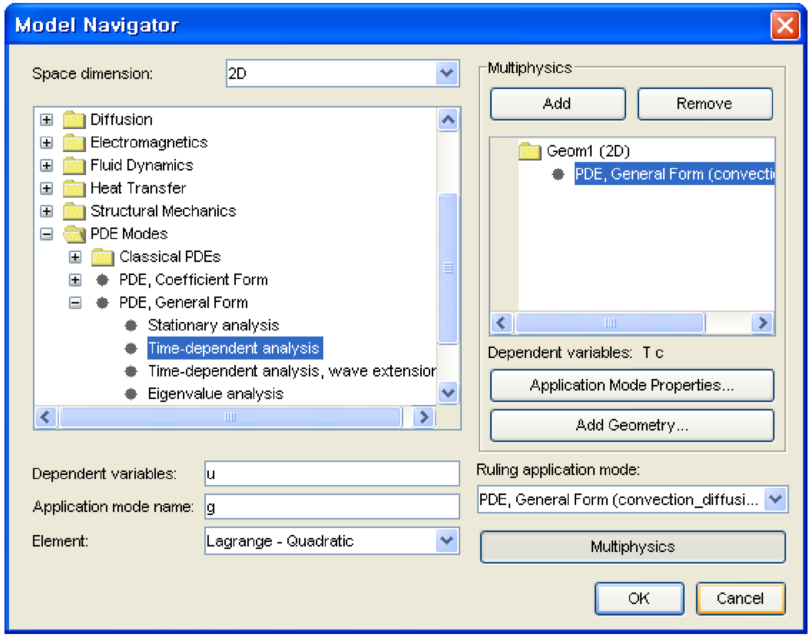
- Parameter conditions

  - r_0=1, r_1=30, r_2=30 $r_1 = \frac{r_2}{r_0}$

    B_1=7.8X10^7, B_2=1.2X10^8 q=17.6

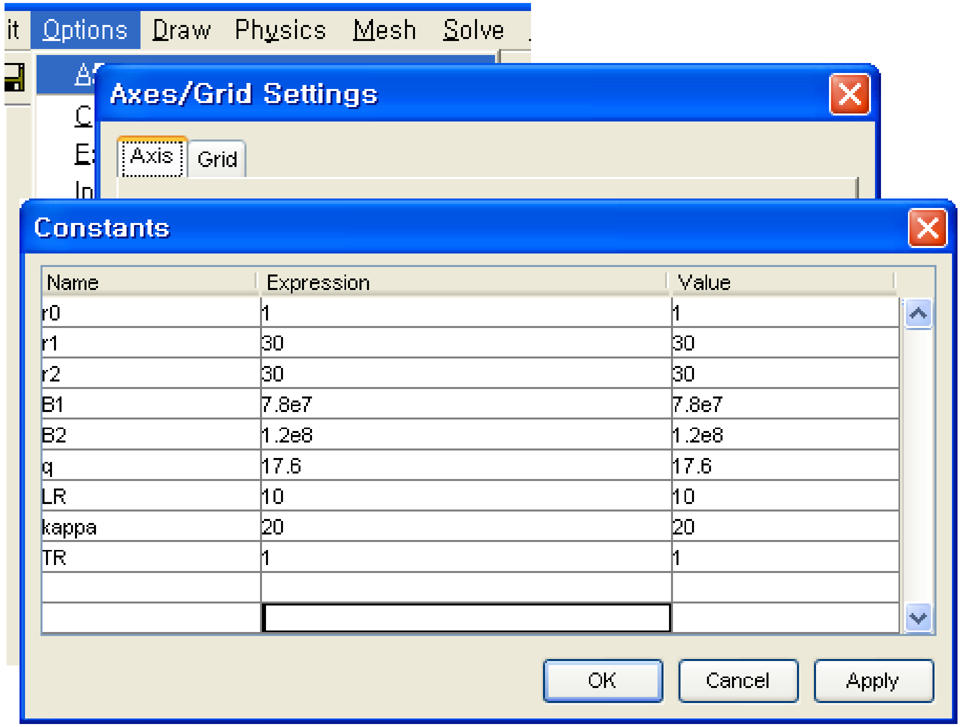
  - T (x,0)=1+0.15x
  - c(x,0)=1
  - L_R=10
  - κ=100
  - T_R=C_0=T_0=1
  - T(x,y,0)=1, c(x,y,0)=1

Model navigator



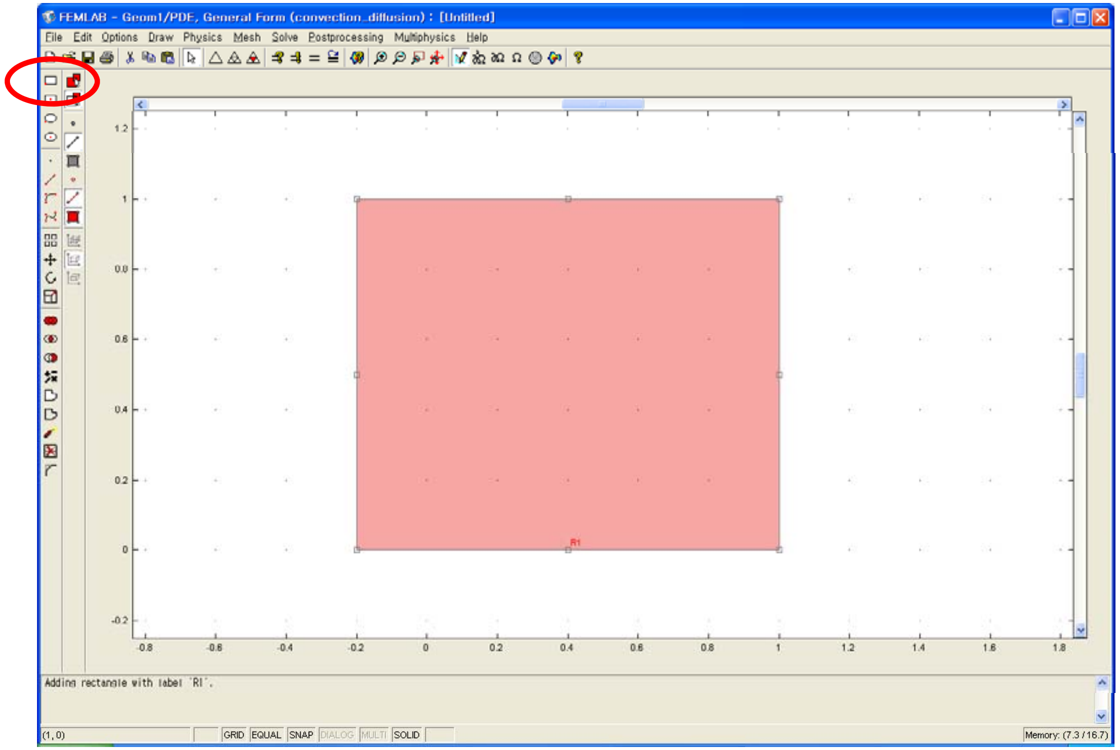
1. In the **Model Navigator**, select **General Time-dependent** from the **PDE modes**.
2. To specify the number of dependent variables, in this case two, enter that value in the edit field for **No. of dependent variables** at the bottom of the **New** page.
3. Select the **Lagrange – Quadratic** element type.
4. Enter T c instead of u in the **Dependent variables** edit field.
5. Change the **Application mode name** to something meaningful, such as convection_diffusion.
6. Press **OK**.

Options and settings



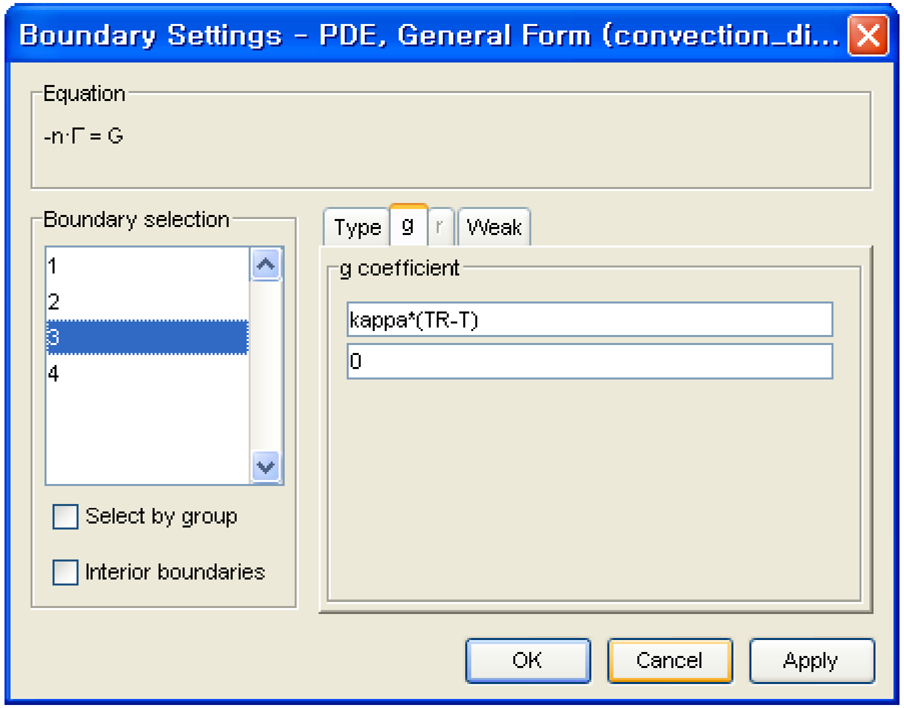
1. Open the **Axis and Grid Settings** dialog box from the **Options** menu. Set the axis limits to [-0.25 1.25] for the x-axis range and [-0.25 1.25] for the y axis range.
2. Open the **Add/Edit Constants** dialog box from the **Options** menu. Enter the following constants. kappa=20 introduces some cooling on the outside of the cylinder.

Geometry modeling



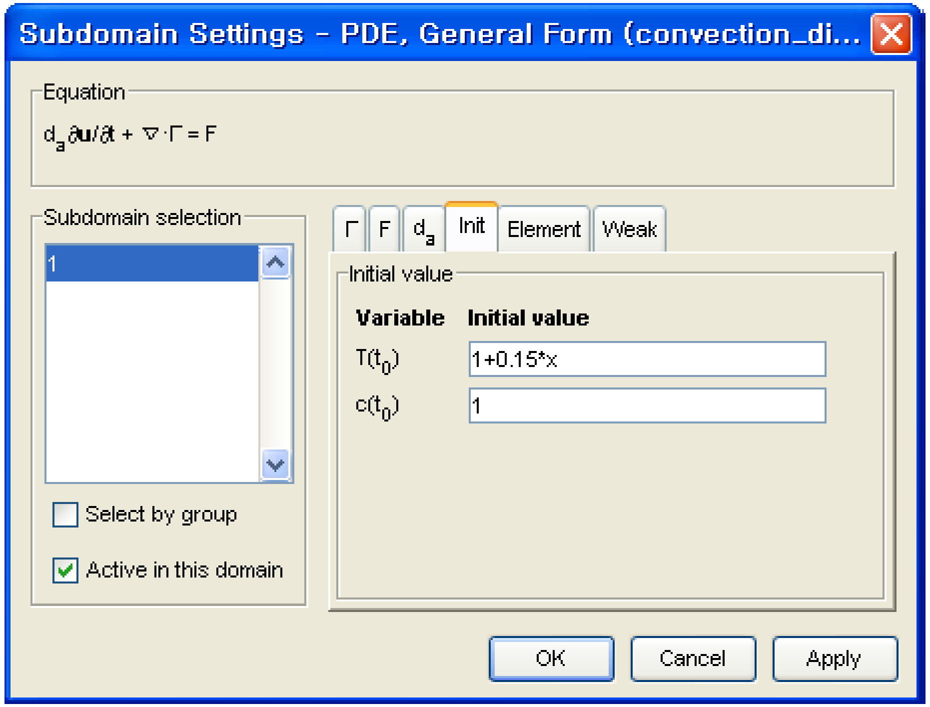
1. Press the **Draw Rectangle** button on the draw toolbar and create a square from the origin to (1, 1).

Physics settings (boundary)



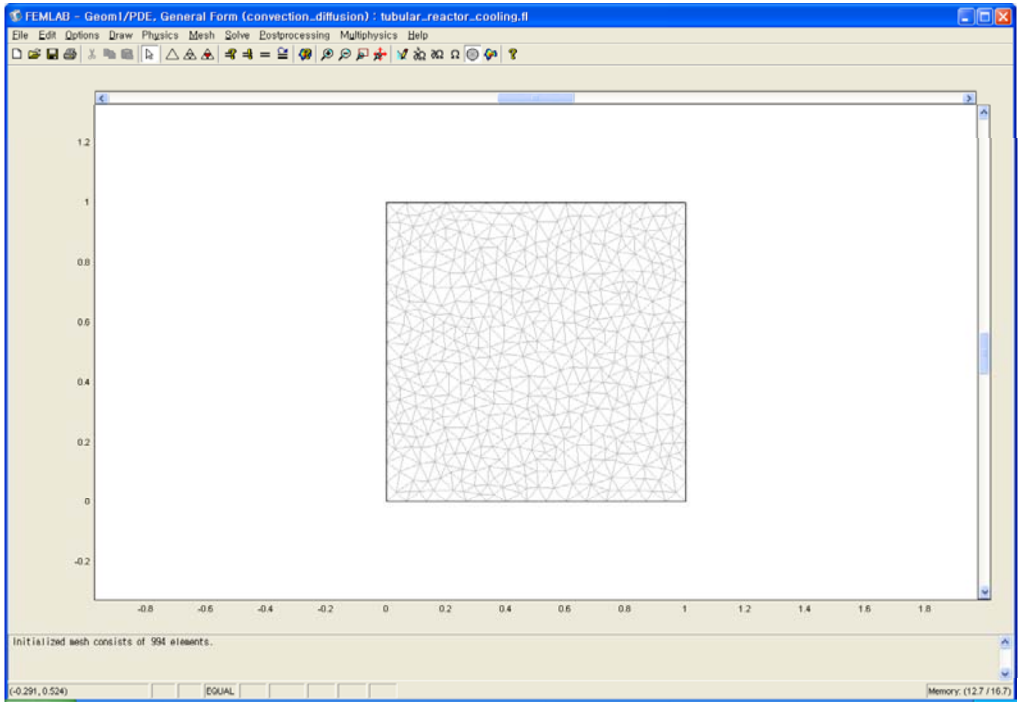
1. Choose **Boundary Settings** from the **Boundary** menu. In the dialog box that opens enter the boundary coefficients as in the following figure.

Physics settings (subdomain)



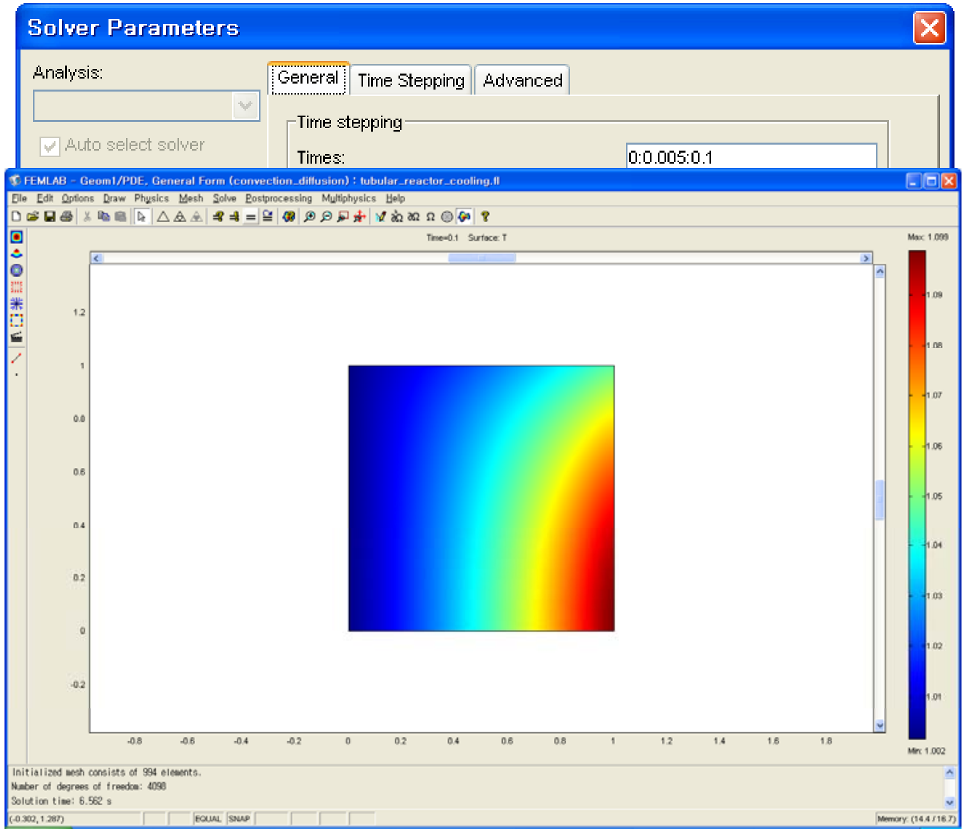
1. Choose **Subdomain Settings** from the **Subdomain** menu. Enter the coefficients from the following figure.
2. Press the **Init** tab in the **Subdomain Settings** dialog box. Set the following initial conditions.

Mesh generation



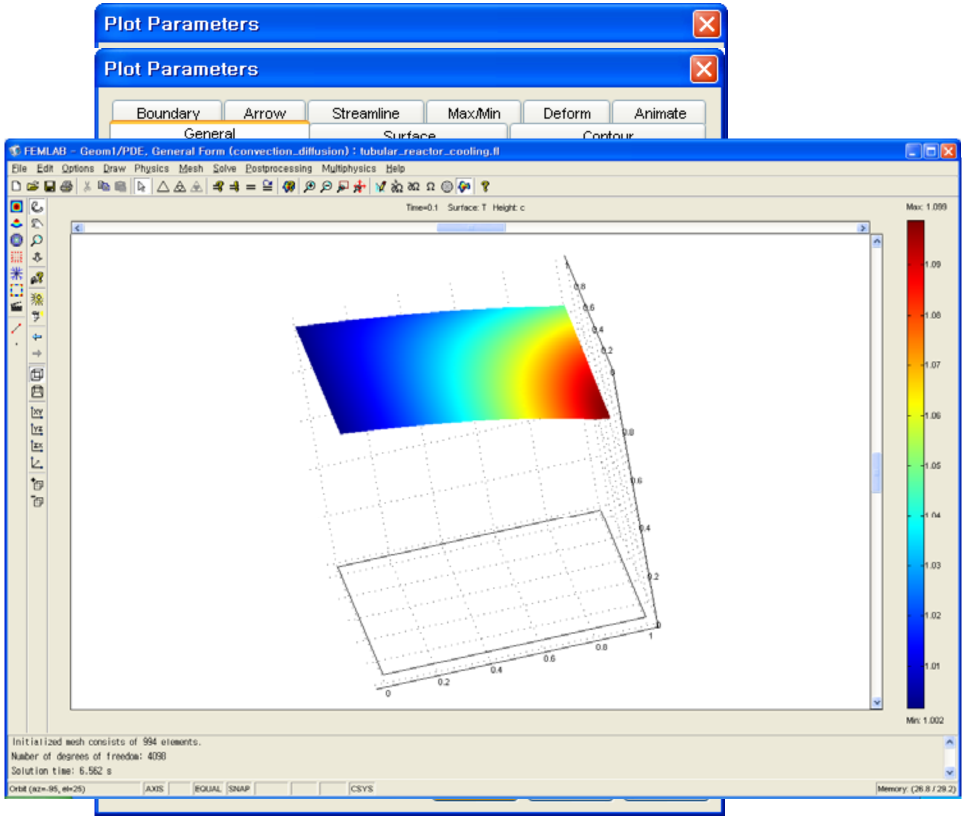
1. Select **Initialize Mesh** from the **Mesh** menu. This action instructs the software to generate and plot an initial mesh.

Solving the model



1. From the **Solve** menu choose **Parameters**, which opens the **Solver Parameters** dialog box. Select the **Time stepping** page and set the time steps to 0:0.005:0.1 in the edit box.
2. Instruct the software to find the solution by going to the **Solve** menu and selecting **Solve Problem** or by pressing the corresponding toolbar button.

Postprocessing and visualization



1. On the **Surface** page in the **Plot Parameters** dialog box, select T for **Surface data** and c for **Height data (3D)**. Press **OK** to see a 3D representation of the variables plotted against each other.
2. Press the **Animation** toolbar button to see how the 3D plot changes over time.
3. On the **General** page, you can examine the solution surface at specific points in time with the **Solution at time** menu.

Conclusions

- As time goes by, cooling effect occurs.